# Convolution-based Particle Tracking for Transient Flows in Porous Media

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Transport in porous media has applications in many physical and biological phenomena such as contaminant transport in groundwater. A popular and effective model for this transport is the ADE. The ADE is a partial differential equation that is derived by modeling the transport processes of advection and dispersion, in combination with the conservation of solute mass. Particle tracking methods offer several advantages over Eulerian discretization approaches for solving the ADE. The CBPT method is an efficient particle-tracking approach that was recently developed for steady-state flows in porous media. This new method needs significantly fewer particles than existing methods, and offers additional efficiencies for sensitivity studies. In this work we extend this to the transient case, and highlight the initial verification tests.

Transport in porous media involves a combination of three passive transport mechanisms: (1) advection due to the groundwater flow driven by pressure gradients, (2) molecular diffusion due to concentration gradients, and (3) hydrodynamic dispersion due to mixing of flow paths of varying velocities as a result of heterogeneities in the medium. Under certain assumptions the continuum approximation is valid, and these processes are accurately modeled by the advection-dispersion equation (ADE). Particle tracking methods are often used to solve the ADE due to their ability to maintain sharp fronts in systems that are advection-dominated or that have strongly anisotropic dispersivity. A drawback of most particle-tracking methods is that producing a sufficiently accurate solution requires a large number of particles, especially with non-point sources and for source terms that vary over time. The Convolution-Based Particle Tracking (CBPT) method [1] is a new, computationally efficient method that calculates plume concentrations by combining particle tracking and convolution, assuming a steady-state flow. In particular, as the duration of the simulated source term increases, the convolution approach is more efficient than traditional Random Walk Particle Tracking (RWPT) techniques. Another advantage of the CBPT method is that a single particle-tracking simulation may be used, through the convolution approach, to efficiently conduct a parametric sensitivity study. However, the CPBT method assumes a steady-state flow, and this is too restrictive. In this work we extend the CBPT method to transient flows.

Standard random walk particle-tracking methods solve the ADE by recognizing its equivalence to the Fokker-Planck equation, and hence, to Ito's interpretation of the corresponding Langevin equation. Transport under steady-state flow conditions can be described by a collection of particle trajectories. Due to the time-invariant nature of the problem, any solute source can be convolved with the obtained trajectories by releasing particles at the initial time. A sufficient number of particles are released at different locations to describe the spatial distribution of solute sources. The details of resident concentration calculations can be found in [1].

In the case of transport in a transient flow field, solute particles entering the domain at different times experience different flow fields. Hence, to accurately describe the temporal nature of the transport, particles must be released at each source location throughout the time domain of transport, such that one may approximate the steady-state flow conditions over each interval of particle release. We compute a separate trajectory for each particle released in each time interval. The interval of particle release depends upon the transients present in the flow; the number of particles released at each time depends on transport parameters such as dispersivity. Each time-varying source is broken into sub-sources, to coincide with the time of particle release. Each of the sub-sources now follows the set of particle trajectories corresponding to those particles released at the start time of the source. The concentration due to each sub-source can be written as a convolution of the mass flux with the trajectories of particles released at the appropriate time. The total concentration is simply the sum of the individual concentrations, obtained by the principle of superposition.

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The test case documented here uses a simple homogeneous 3D moel with flow along the x direction. The domain (10 km × 600 m × 600 m) is discretized uniformly with 100-m grid spacing in all directions. The flux at the inlet is prescribed and a constant head boundary is applied on the downstream plane. No flow conditions are assumed on the other sides. The solute mass is input into the domain at the upstream end as a point source, centered in the middle of the *y-z* plane. The model described here is advection-only transport for linearly increasing flow with time. In order to capture the temporal variations in the flow, 1200 particles are released uniformly over 300 days.

The results for the concentrations obtained from the CBPT method are verified by both semi-analytical and numerical (RWPT) techniques in [2]. The RWPT calculation used 10,000 particles released uniformly over 300 days in the process model run. The plume at several times is shown in Fig. 1 for both the CBPT and RWPT methods. Since the flow is linearly increasing, and the mass flux at the inlet is fixed, the concentration at the inlet decreases with time, while the concentration profile is monotonically increasing. Figure 1 also shows that sharp fronts, which are characteristic of advection-dominated transport, are maintained at all times. Using the concentration computed with the semi-analytical method as a reference, the error in the CBPT concentration has a maximum of $9.6\times10^{-8}$ mol/l.

These calculations of plume concentration are composed of two parts, the computation of the flow field, and the particle tracking. Since the computational cost of particle tracking is directly proportional to the number of particles, the CBPT method is approximately 10 times faster than the RWPT method. The overall speedup depends on the cost of the flow calculation. Additionally the convolution step in CBPT is approximately 100 times faster than the RWPT method. This step in the calculation can reuse the particle trajectories obtained previously to conduct parameter studies, including time-varying sources and radioactive decay constants, very efficiently. This feature is a significant computational advantage for Monte Carlo-based analysis of transport uncertainty.

We have developed the transient CBPT method and shown that it requires fewer particles in the underlying particle tracking process model run to obtain similar or greater accuracy than traditional RWPT techniques. In addition, particle trajectories are independent, so the total number of particles can be distributed across many processor cores, and the particle tracking executed in parallel.

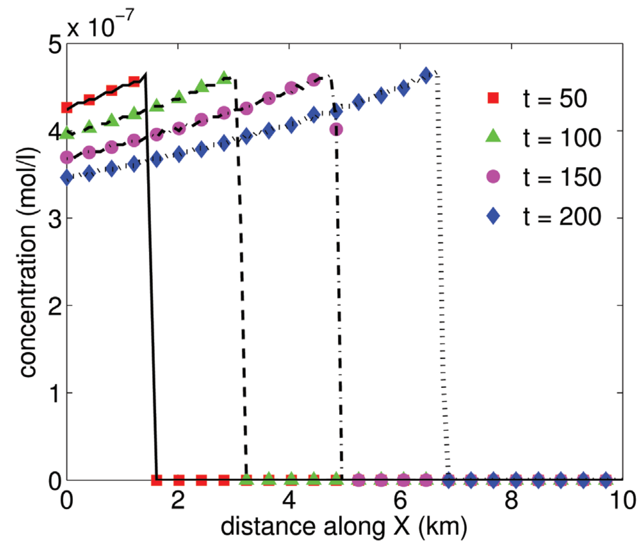


*Fig. 1. The 1D plume for a linearly increasing flow with constant continuous source for advective transport at different times. CBPT (symbols) results are in excellent agreement with the RWPT (lines) results.*

[1] Robinson, B.A., et al., *Comput Geosci* **14,** 779 (2010).
[2] Srinivasan, G., et al., *Water Resour Res,* submitted (2010).

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